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Dynamics of Observed Reality: Abridged Version of Classical and Quantum Mechanics

by

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DYNAMICS OF OBSERVED REALITY: ABRIDGED VERSION OF CLASSICAL AND QUANTUM MECHANICS

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INTRODUCTION

The present paper is concerned with a unified description of classical and quantum physics. A different way of thinking about the quantum world is expounded, which already has led to significant results in statistical mechanics and holds future promise for quantum mechanics. An explanation is provided for the original motivation in quantum theory, the formalisms that have evolved from it and their differences with the classical theories. The conceptual difficulty that permeates our view of the microscopic world is spelled out and a remedy thereof suggested.

BACKGROUND

The laws of nature for the microscopic world are very much different from those of the macroscopic world, though the building blocks of any macroscopic system are the microscopic particles. Notable differences are: (1) Indeterminism in classical statistical mechanics merely reflects our ignorance of initial conditions. In the quantum world indeterminism seems to be unavoidable even in principle. (2) Unlike classical mechanics, quantum mechanics makes explicit conflict between the dynamical description and the process of measurement. Dynamical equations for microscopic systems are based on objective reality and are reversible in time, as are the equations of classical dynamics. However, the observed reality -- the irreversibility of the microworld -- is an outcome of measurement and thus directly conflicts with the objective reality. (3) Bose-Einstein (BE) and Fermi-Dirac (FD) statistics incorporate quantum uncertainty through the indistinguishability of the particles with respect to their coordinates. This gives rise to exchange terms in quantum statistical mechanics. There is no analogue of exchange terms in classical statistical mechanics. (4) Many particle wavefunctions for the microworld obey certain symmetry rules. This quantum mechanical limitation has no immediate counterpart in classical statistics.

One possible way to resolve these conflicts would be to abandon the objective reality, as advocated by the believers of the Copenhagen

interpretation [1]. The quantum Liouville equation for mixtures, which describes the dynamics of observed reality for the microworld, would then be an appropriate dynamical equation. The central task is thus the evaluation of the quantum distribution function (QDF), because the QDFs provide a means of expressing quantum mechanical averages in a form which is very similar to that for classical averages [2]. This is the case with the Ehrenfest representation (ER), where a correspondence between a classical trajectory and the expectation values of the corresponding quantum operators is established [3]. However, in most cases, including ER, the equations of motion for the average values of position, momentum, etc. are not closed and therefore cannot be solved without further assumptions. Moreover, attempts to write a proper QDF that is positive and gives the correct individual quantum distributions of position and momentum have been in vain [2,4]. It is suspected that the quantum mechanical uncertainty and the noncommutativity of position and momentum prohibits a phase space construction of the QDFs. For these reasons, it has not been possible to develop theories for the microworld based on observed reality. However, in recent years, it has been found that the Wigner transforms of all the Gaussian QDFs are non-negative, corresponding to pure states and mixtures [5]. Existence of such phase space QDFs gives us an opportunity to study the dynamics of the microscopic world based on observed reality. This is what constitutes the main content of the present paper.

Our system of investigation is an N-particle statistical system whose time evolution is described by the quantum Liouville equation for mixtures [6]. We focus on studying the dynamics of each single particle in the N-particle ensemble. We do not assume <u>a priori</u> that the indistinguishability of the particles is necessary when their de Broglie wavelengths ($\bar{\lambda}$) are greater than or equal to their mean distances ($\bar{R}$). Instead, we measure the quantum uncertainties associated with each particle in order to understand whether indistinguishability is inherent in microscopic many-particle systems. The development is based on constructing a Gaussian density matrix in three-dimensional phase space. The density matrix is defined by a set of dynamical variables whose expectation values are considered to be relevant for the dynamics. Construction of the density function is based on a maximum entropy formulation [7], and our choice of the dynamical variables is reflected in such construction. The self-consistent equations of motion are then derived for these expectations from the quantum Liouville equation using a projection scheme [8,9]. The solution of these self-consistent field (SCF) equations provides the time evolution of the density matrix.

In the next section we derive the equations of motion for the expectations of these dynamical quantities and construct the corresponding density function for mixed states. We also show that these equations of motion can be derived solving the classical Liouville equation for mixtures. In Sec. III we show that for systems in thermal equilibrium these equations satisfy a new principle of least action. Again, a simple combination of classical and quantum laws can be used to generate these equations. Finally, in Sec. IV we discuss the relative merits of the theories based on observed reality with those of objective reality.

DERIVATION OF THE BASIC EQUATIONS SOLVING QUANTUM LIOUVILLE EQUATION AND CONSTRUCTION OF THE DENSITY FUNCTION

We characterize our N-particle system by the Hamiltonian

$$H = \sum_{k=1}^{N} \frac{p_k^2}{2m_k} + V(r_1 \ldots r_N) \qquad (1)$$

and a density matrix $\rho(R,R';t)$ which satisfies the quantum Liouville equation (QLE)

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H,\rho] \equiv -iL\rho \quad , \qquad (2)$$

where V is the interaction potential and m_k is the mass of the k-th particle, r_k is the coordinate of the k-th particle, and $p_k = \frac{\hbar}{i}\nabla_k$ is its conjugate momentum. We are interested in an approximate solution of the QLE where the time evolution of the exact N-particle system is described by a reduced density matrix $\rho_{re}(R,R';t)$, which is a product of N single particle density functions,

$$\rho_{re}(R,R';t) = \prod_{i=1}^{N} \phi_j(r_j,r_j';t) \quad , \qquad (3)$$

where R is a vector with N coordinate components $r_1 \ldots r_N$. This choice [Eq. (3)] of the density function excludes the possibility of incorporating quantum uncertainty into our system through the indistinguishability of the particles with respect to their coordinates. We introduce the effect of quantum uncertainty by characterizing each particle with respect to its position, momentum and their fluctuations. For this reason, we define each particle in three dimensions using a set of operators, O_α, $\alpha = 1,\ldots, M$, which are x_k, $\hat{p}_k$, $\hat{x}_k\hat{x}_\ell$, $\hat{p}_k\hat{p}_\ell$ and $\hat{x}_k\hat{p}_\ell$, for $k,\ell = 1, 2, 3$. In general, to describe the dynamics of each particle in three dimensions (3D) incorporating quantum uncertainties, we need $M = 2.3^2 + 3.3 = 27$ independent operators consisting of a complete set of linear and bilinear products of $\hat{x}_k$ and $\hat{p}_k$. For notational convenience, we shall represent these operators in the following matrix form:

$$A_0 = 1 \quad , \quad A_1 = \hat{r} \quad , \quad A_2 = \hat{p}$$

$$A_3 = (\hat{r} - \sigma_1)\cdot(\hat{r} - \sigma_1)^T \quad , \quad A_4 = (\hat{p} - \sigma_2)\cdot(\hat{p} - \sigma_2)^T$$

$$A_5 = (\hat{r} - \sigma_1)\cdot(p - \sigma_2)^T - \frac{1}{2}\hbar I \quad . \qquad (4)$$

Here, A_0 is the unit operator; A_1 and A_2 are three component vectors; A_3, A_4 and A_5 are 3×3 matrices and I is the 3×3 unit matrix; σ_1 and σ_2 are the expectation values of the dynamical quantities A_1 and A_2; and the superscript T stands for transpose. The time evolution of the expectations of these dynamical quantities, $\langle A_i \rangle$'s, will provide us with the average values of position ($\langle A_1 \rangle$), momentum ($\langle A_2 \rangle$), and their fluctuations (diagonal terms of $\langle A_3 \rangle$ and $\langle A_4 \rangle$) and correlations (off-diagonal terms of $\langle A_3 \rangle$ and $\langle A_4 \rangle$ and $\langle A_5 \rangle$). $\langle A_5 \rangle$ has the unit of action, and the role of its diagonal elements in the present dynamical description will be discussed later. Here, we should note that $\langle A_3 \rangle$ and $\langle A_4 \rangle$ are symmetric matrices.

To derive explicit expressions for the time evolution of the expectations, $\langle O_{j\alpha}(t) \rangle$, for each particle j, we use a projection operator technique in Liouville space [8,9]. In this space, $\hat{H}$ and $\rho(t)$ can be written as $|H\rangle\rangle$ and $|\rho(t)\rangle\rangle$. Since the exact density matrix $\rho(t)$ contains information more than required by the present method, we evaluate expectation values of the dynamical quantities $O_{j\alpha}$ using

Codes
A-1

$$a_{j\alpha}(t) \equiv \langle\langle 0_{j\alpha}|\rho(t)\rangle\rangle = \langle\langle 0_{j\alpha}|\rho_{re}(t)\rangle\rangle \qquad \alpha = 0, 1, \ldots, M \quad . \tag{5}$$

For each degree of freedom j, we now define an (M+1)×(M+1) overlap matrix with elements

$$D^j_{\alpha\beta} = \langle\langle 0_{j\alpha}|\rho_{re}(t)\, 0_{j\beta}\rangle\rangle$$
$$= \mathrm{Tr}\,[0^\dagger_{j\alpha}\, \rho_{re}(t)\, 0_{j\beta}] \qquad \alpha, \beta = 0, 1, \ldots, M \tag{6}$$

and the Liouville space projection operators

$$P(t) = \sum_{j=1}^{N} \sum_{\alpha,\beta=0}^{M} |\rho_{re}(t)0_{j\alpha}\rangle\rangle [D^j(t)]^{-1}_{\alpha\beta} \langle\langle 0_{j\beta}| \quad . \tag{7}$$

The properties of the above projection operator have been discussed in Refs. 8 and 9. Let us now assume that at some time $t = t'$

$$\rho(t') = \rho_{re}(t') \quad . \tag{8}$$

Introducing the complementary projection $Q(t) = 1 - P(t)$, along with the projection operator properties discussed in Refs. 8 and 9, we can then derive the equations of motion for the $0_{j\alpha}(t)$'s from the QLE in the form [9]

$$\dot{a}_{j\alpha}(t) = -i\langle\langle 0_{j\alpha}|L|\rho_{re}(t)\rangle\rangle + \sum_{\beta} M^j_{\alpha\beta}(t,t')\, a_{j\beta}(t) \quad , \tag{9a}$$

where $M^j_{\alpha\beta}(t,t')$ is expressed in terms of the 28×28 matrices

$$W^j_{\alpha\beta}(t,t') = -i\langle\langle 0_{j\alpha}|LQ(t)U(t,t')|\rho_{re}(t')0_{j\beta}\rangle\rangle \quad , \tag{9b}$$

$$R^j_{\alpha\beta}(t,t') = \langle\langle 0_{j\alpha}|U(t,t')|\rho_{re}(t')0_{j\beta}\rangle\rangle \tag{9c}$$

and is given by

$$M^j_{\alpha\beta}(t,t') = \sum_{\gamma=0}^{M} W^j_{\alpha\gamma}(t,t')[R^j(t,t')]^{-1}_{\gamma\beta} \quad . \tag{9d}$$

Here $U(t,t')$ is the time evolution operator

$$U(t,t') = \exp[-iL(t-t')] \quad . \tag{9e}$$

Equations (9) describe the time evolution of the 27N dynamical quantities ($j = 1, 2, \ldots, N$; $\alpha = 1, 2, \ldots, 27$) and are exact. These equations are closed for 27N unknown $a_{j\alpha}(t)$'s. In these equations, the time derivative of $a_{j\alpha}(t)$ at time t depends on all $a_{j\beta}(t)$ at the same time. Note that we assume 0_{j0} to be the unit operator and the normalization condition requires its expectation values to be independent of time, $a_{j0} = 1$. Now if we assume that condition (8) holds for all times, then $Q(t)\rho(t) = 0$ and we are left with the first term on the right-hand side of Eq. (9a), which represents a mean-field time evolution of the N-particle system, where the time evolution of the expectations of the dynamical quantities, $0_{j\alpha}$, are given by

$$\dot{a}_{j\alpha}(t) = -\frac{i}{\hbar}\,\mathrm{Tr}\{0_{j\alpha}[H,\rho_{re}(t)]\} \equiv -i\langle\langle 0_{j\alpha}|L|\rho_{re}(t)\rangle\rangle \quad . \tag{10}$$

Equation (10) describes the time evolution of the dynamical quantities $\hat{x}_k$, $\hat{P}_k$, $\hat{x}_k\hat{x}_\ell$, $\hat{P}_k\hat{P}_\ell$ and $\hat{x}_k\hat{P}_\ell$ for $k,\ell = 1, 2, 3$.

To determine directly the quantum uncertainties associated with each particle, we evaluate explicitly the time evolution of the dynamical quantities

$$\sigma_1 = <\hat{r}> \quad , \quad \sigma_2 = <\hat{p}> \tag{11a,b}$$

$$\sigma_3 = <(\hat{r} - \sigma_1)\cdot(\hat{r} - \sigma_1)^T> \tag{11c}$$

$$\sigma_4 = <(\hat{p} - \sigma_2)\cdot(\hat{p} - \sigma_2)^T> \tag{11d}$$

$$\sigma_5 = <(\hat{r} - \sigma_1)\cdot(\hat{p} - \sigma_2)^T> - \tfrac{1}{2}\hbar I \tag{11e}$$

given by

$$\dot{\sigma}_1 = \Lambda\sigma_2 \tag{12a}$$

$$\dot{\sigma}_2 = - V' \tag{12b}$$

$$\dot{\sigma}_3 = \sigma_5\Lambda + \Lambda\sigma_5^T \tag{12c}$$

$$\dot{\sigma}_4 = - V''\sigma_5 - \sigma_5^T V'' \tag{12d}$$

$$\dot{\sigma}_5 = - \sigma_3 V'' + \Lambda\sigma_4 \quad , \tag{12e}$$

where

$$V' = <\frac{\partial V}{\partial r}> \quad , \quad V'' = <\frac{\partial^2 V}{\partial r\cdot\partial r^T}> \quad , \quad \Lambda = m^{-1}I \quad . \tag{13}$$

Equations (12) describe time evolution of 27 matrix elements which are the expectations of the physical operators described by Eq. (4). σ_α for $\alpha = 1, 2, \ldots, M$ are

$$\sigma_{1k}(t) = <x_k> \quad , \quad \sigma_{2k}(t) = <p_k> \tag{14a,b}$$

$$[\sigma_3(t)]_{k\ell} = <[x_k - \sigma_{1k}(t)][x_\ell - \sigma_{1\ell}(t)]> \tag{14c}$$

$$[\sigma_4(t)]_{k\ell} = <[p_k - \sigma_{2k}(t)][p_\ell - \sigma_{2\ell}(t)]> \tag{14d}$$

$$[\sigma_5(t)]_{k\ell} = \frac{1}{2} <[\hat{x}_k - \sigma_{1k}(t)][\hat{p}_\ell - \sigma_{2\ell}(t)] + [\hat{p}_\ell - \sigma_{2\ell}(t)][\hat{x}_k - \sigma_{1k}(t)]> \tag{14e}$$

$$k,\ell = 1, 2, 3 \quad .$$

These expectation values in quantum mechanics are evaluated either in the coordinate (r,r') or momentum (p,p') representation.

From Eq. (12), we find that for a successful application of the present method, the choice of ϕ_j is crucial. We construct each ϕ_j from the physical consideration which is the maximum entropy principle [7]. We associate entropy with each particle using the relation

$$S = - k\, Tr[\phi_j\, \ell n\phi_j] \quad . \tag{15a}$$

We then maximize entropy ($\delta S = 0$) subject to the constraint condition

$$\delta a_\alpha(t) = \mathrm{Tr}[0_\alpha \, \delta\phi_j] = 0 \qquad \alpha = 0, 1, \ldots, M \quad . \tag{15b}$$

This yields the maximum entropy distribution

$$\phi_j(t) = \exp\Big[\sum_{\alpha=0} - \lambda_{j\alpha}(t) 0_{j\alpha}\Big] \quad , \tag{16}$$

where the $\lambda_{j\alpha}(t)$'s are Lagrange multipliers and describe the time evolution of the density function ϕ_j. This distribution function is Gaussian in 3D-phase space $(q,p)_j$ and in the corresponding coordinate representation (r,r'), whose explicit forms are given by

$$\begin{aligned}\phi(r,r';t) = C \exp\{ &- \tfrac{1}{2}[\tfrac{1}{4}(r+r')^T \sigma_3^{-1}(r+r') - \tfrac{2}{i\hbar}(r-r')^T(\sigma_5^T\sigma_3^{-1}\sigma_1 - \sigma_2) \\ &+ \tfrac{1}{\hbar^2}(r-r')^T(\sigma_4 - \sigma_5^T\sigma_3^{-1}\sigma_5)(r-r') \\ &+ \tfrac{1}{i\hbar}(r+r')^T \sigma_3^{-1}\sigma_5(r-r') - (r+r')^T\sigma_3^{-1}\sigma_1]\}\end{aligned} \tag{17a}$$

with

$$C = (2\pi)^{-3/2} \, \|\sigma_3\|^{-1/2} \exp[-\tfrac{1}{2}\sigma_1^T\sigma_3^{-1}\sigma_1] \quad , \tag{17b}$$

and

$$\phi(q,p;t) = (2\pi)^{-3} \, \|B\|^{-1/2} \exp\{-\tfrac{1}{2}[(q^T - \sigma_1^T) \, , \, (p^T - \sigma_2^T)] \, B^{-1} \begin{bmatrix} q - \sigma_1 \\ p - \sigma_2 \end{bmatrix}\} \quad , \tag{18a}$$

where B is a matrix given as

$$B = \begin{bmatrix} \sigma_3 & \sigma_5 \\ \sigma_5^T & \sigma_4 \end{bmatrix} \quad . \tag{18b}$$

$\phi(q,p;t)$ is obtained form $\phi(r,r';t)$ using the Wigner transform [2]

$$\phi(q,p;t) = \frac{1}{(\pi\hbar)^3} \iiint_{-\infty}^{\infty} ds \, \langle q-s|\hat{\phi}(t)|q+s\rangle e^{2ip\cdot s/\hbar} \tag{19a}$$

and satisfies

$$\iint_{-\infty}^{\infty} dq \, dp \, \phi(q,p;t) = 1 \quad . \tag{19b}$$

Therefore, the expectation values of the dynamical quantities [Eq. (11)] in the present method can be evaluated using both the trace operation (r,r') and the phase space (q,p) integration methods. The time evolution of these density functions are obtained by solving the coupled set of equations (12). A close look at these equations shows that they do not contain $\hbar$. This suggests that they are completely classical. In fact, we obtained these TDSCF set of equations (12) also by solving the classical Liouville equation using the phase space distribution function (18), and following the same procedure discussed above. The TDSCF set of equations

for the moments $\sigma_1, \ldots, \sigma_5$ using Gaussian distribution functions are therefore completely classical.

The present classical set of equations (12) differ from Ehrenfest's representation due to the fact that they contain additional dynamical quantities (σ_3, σ_4 and σ_5) and are closed. To understand the potentiality of the present method, we need extensive application. So far, we have studied only the equilibrium properties of liquid and solid argon, assuming the system to be isotropic. The results of this simulation have been reported in a separate communication [10]. Here we elucidate only the underlying physics. Of the various dynamical quantities, only the time evolution of $\sigma_5(t)$, which has the unit of action, shows rapid oscillations between positive and negative values. This time dependence of $\sigma_5(t)$ implies that at different times of the measurement each particle has a different trajectory, which in turn suggests that the classical trajectory obtained solving (12) does not satisfy the principle of least action [11]. The time evolution of this $\sigma_5(t)$ is shown in Fig. 1. From this figure, we find that the time-averaged trajectory for systems in thermal equilibrium has $\sigma_5 = 0$. Since our system of investigation is isotropic, $[\sigma_5]_{ij}$ for $i \neq j$ remains zero over all times. Now substituting $\langle A_5 \rangle = 0$ in Eq. (12),

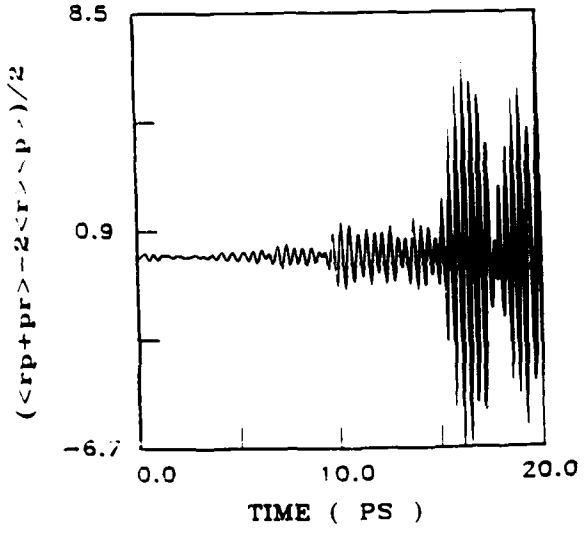

Fig. 1. Time evolution of the action, $\sigma_5(t) = \sum_{i=1}^{3} \sigma_5^i(t)$ for i = x, y and z over 20 ps in a typical run for solid argon (V_m = 28.096, T = 50.275 K). $\sigma_5^i(t)$ is the action along the i-th direction of phase space and averaged over the entire bath. The value of $\sigma_5(t)$ originally in kg $m^{-2} s^{-1}$ has been magnified 10^{36} times in this figure.

$$\dot{\sigma}_1 = \Lambda\sigma_2 \qquad (20a)$$

$$\dot{\sigma}_2 = -V' \qquad (20b)$$

$$\dot{\sigma}_3 = 0 \qquad (20c)$$

$$\dot{\sigma}_4 = 0 \quad . \qquad (20d)$$

That is, for systems in thermal equilibrium, the fluctuations σ_3 and σ_4 are the constants of motion. In the following section, we show that Eq. (20) can be obtained using a modified representation of the classical principle of least action and also from a simple combination of the Ehrenfest representation with the equations of motion derived from the quantum uncertainty principle.

ALTERNATIVE APPROACHES TO THE DERIVATION OF THE BASIC EQUATIONS FOR SYSTEMS IN THERMAL EQUILIBRIUM

Principle of Least Action

We introduce the following principle of least action for each particle in the N-particle ensemble:

$$\sigma_5^j = \int_{t_a}^{t_b} dt \, \langle \hat{L}_j \rangle \qquad j = 1, 2, \ldots, N \quad . \tag{21}$$

Here $\hat{L}_j$ is the Lagrange operator for the j-th particle and

$$\hat{L}_j = \sum_{k=1}^{3} \frac{\hat{p}_{jk}^2}{2m_j} + \hat{V}_j(R) \quad , \tag{22}$$

where its quantum average is

$$L_j = \langle \hat{L}_j \rangle = \frac{1}{2m_j} \sum_{k=1}^{3} \{(\sigma_{2k})^2 + [\sigma_4]_{kk}\}_j - \int_{-\infty}^{\infty} dR \, V_j(R) \, \rho_{re}(R,R;t) \quad , \tag{23}$$

and the $\sigma_{k\ell}$'s are defined in Eq. (14). Let us now assume that the extremum path for the ℓ-th particle is defined by $\bar{\sigma}_1^{\ell}(t)$, whose end points are $\sigma_1^{\ell}(t_a)$ and $\sigma_1^{\ell}(t_b)$. In 3D phase space

$$\sigma_1^{\ell} = i\langle x^{\ell} \rangle + j\langle y^{\ell} \rangle + k\langle z^{\ell} \rangle = i\sigma_{11}^{\ell} + j\sigma_{12}^{\ell} + k\sigma_{13}^{\ell} \quad . \tag{24}$$

To determine the form of this path, we use the usual procedure of the calculus of variations.

Let us assume that the path is varied away from $\bar{\sigma}_1^{\ell}(t)$ by an amount $\delta\sigma_1^{\ell}(t)$, with the condition that the end points are fixed, that is,

$$\delta\sigma_1^{\ell}(t_a) = \delta\sigma_1^{\ell}(t_b) = 0 \quad . \tag{25}$$

Now the condition that $\bar{\sigma}_1^{\ell}(t)$ be an extremum means

$$\delta\sigma_5^{\ell} = \sigma_5^{\ell}[\bar{\sigma}_1^{\ell} + \delta\sigma_1^{\ell}] - \sigma_5^{\ell}[\bar{\sigma}_1^{\ell}] = 0 \tag{26}$$

to first order in $\delta\sigma_1^{\ell}$. Using the definitions (21) and (23), we may write

$$\begin{aligned} \sigma_5^{\ell}[\sigma_1^{\ell} + \delta\sigma_1^{\ell}] = & \int_{t_a}^{t_b} dt \, L_{\ell}(\sigma_1^{\ell} + \delta\sigma_1^{\ell}, \, \sigma_2^{\ell} + \delta\sigma_2^{\ell}, \, \sigma_3^{\ell} + \delta\sigma_3^{\ell}, \, \sigma_4^{\ell} + \delta\sigma_4^{\ell}) \\ & - \sigma_5^{\ell}[\bar{\sigma}_1^{\ell}] + \int_{t_a}^{t_b} dt \, [\delta\sigma_1^{\ell} \frac{\partial L_{\ell}}{\partial \sigma_1^{\ell}} + \delta\sigma_2^{\ell} \frac{\partial L_{\ell}}{\partial \sigma_2^{\ell}} \\ & + \delta\sigma_3^{\ell} \frac{\partial L_{\ell}}{\partial \sigma_3^{\ell}} + \delta\sigma_4^{\ell} \frac{\partial L_{\ell}}{\partial \sigma_4^{\ell}}] \quad , \end{aligned} \tag{27}$$

where, for example, $\partial L_{\ell}/\partial\sigma_1^{\ell}$ implies variation of L_{ℓ} with respect to all the q_{ik}^{ℓ} elements (k = 1, 2, 3). Upon integration by parts, the variation in σ_5^{ℓ} becomes

$$\delta\sigma_5^{\ell} = m_{\ell} \, \delta\sigma_1^{\ell} \frac{\partial L_{\ell}}{\partial \sigma_2^{\ell}} \Big|_{t_a}^{t_b} - \int_{t_a}^{t_b} dt \, \{\delta\sigma_1^{\ell}[m_{\ell} \frac{d}{dt}(\frac{\partial L_{\ell}}{\partial \sigma_2^{\ell}})$$

$$- \frac{\partial L_\ell}{\partial \sigma_1^\ell}] + \delta\sigma_3^\ell \frac{\partial L_\ell}{\partial \sigma_3^\ell} + \delta\sigma_4^\ell \frac{\partial L_\ell}{\partial \sigma_4^\ell}) \quad . \tag{28}$$

The first term on the right-hand side of this equation is zero since $\delta\sigma_1^\ell$ is zero at the end points. The second term is zero if the following condition is satisfied:

$$\delta\sigma_1^\ell [\frac{d}{dt}(\frac{\partial L_\ell}{\partial \dot{\sigma}_1^\ell}) - \frac{\partial L_\ell}{\partial \sigma_1^\ell}] + \delta\sigma_3^\ell \frac{\partial L_\ell}{\partial \sigma_3^\ell} + \delta\sigma_4^\ell \frac{\partial L_\ell}{\partial \sigma_4^\ell} = 0 \quad . \tag{29}$$

Since the variation of L_ℓ with respect to σ_1^ℓ and σ_3^ℓ contains σ_1^k and σ_3^k for $k \neq \ell$, to obtain the extremum path for each particle we need to solve 3N coupled equations obtained from the variation of σ_ξ^ℓ ($\ell = 1, 2, \ldots, N$). In the following, we shall show that Eq. (20) can result from a trivial solution of these 3N coupled equations. Since between the end points $\delta\sigma_1^\ell$ can take any arbitrary value, the first term in Eq. (29) is zero provided

$$\frac{d}{dt}(\frac{\partial L_\ell}{\partial \dot{\sigma}_1^\ell}) - \frac{\partial L_\ell}{\partial \sigma_1^\ell} = 0 \quad . \tag{30}$$

These are the Langrange equations of motion for the quantum-averaged dynamical quantities $\sigma_1^\ell(t)$ and $\sigma_2^\ell(t)$. The second and third terms in Eq. (29) can only be zero if

$$\delta\sigma_3^\ell = \delta\sigma_4^\ell = 0 \quad . \tag{31}$$

This is because, is we differentiate L_ℓ of Eq. (23) with respect to σ_3^ℓ and σ_4^ℓ, then

$$\frac{\partial L_\ell}{\partial \sigma_3^\ell} = - \frac{\partial}{\partial \sigma_3^\ell} \langle V_\ell(R) \rangle \neq 0 \quad , \quad \frac{\partial L_\ell}{\partial \sigma_4^\ell} = \frac{1}{m_\ell} \quad . \tag{32}$$

Solving the Lagrange equations (30), we obtain Eqs. (20a,b), and from the condition (31) we obtain Eqs. (20c,d). Thus, a trivial solution of the 3N coupled equations shows that there is a principle of least action (21), from which Eq. (20) can be obtained. In the following subsection, we show that Eq. (20) can be derived by combining the Ehrenfest representation with the equations of motion for the fluctuations obtained from the quantum uncertainty principle.

Extension of the Ehrenfest Representation

Ehrenfest's equations describe the time evolution of the mean values of the coordinates $\langle x \rangle$ and momenta $\langle p \rangle$. With the Hamiltonian given by Eq. (1), the time evolution of these expectations may be written as

$$\frac{d}{dt}\langle x_j \rangle = \langle \frac{\partial H}{\partial p_j} \rangle = \langle p_j/m \rangle \qquad j = 1, 2, \ldots, 3N \tag{33a}$$

$$\frac{d}{dt}\langle p_j \rangle = - \langle \frac{\partial H}{\partial x_j} \rangle = - \langle V_j'(R) \rangle \qquad j = 1, 2, \ldots, 3N \quad . \tag{33b}$$

These equations do not follow the classical laws of motion due to the fact that the time derivatives of $\langle x_j \rangle$ and $\langle p_j \rangle$ are equal to certain average values whose calculation generally necessitates the knowledge of the wavefunction $\Psi(t)$. Our TDSCF equations, (20a,b), are identical to these equations, except that the average values are evaluated using a density

function $\rho_{re}(t)$. Ehrenfest's equations may thus be viewed as a special case of our TDSCF set of equations (20), where the contributions of the fluctuations are not taken into account and the density function represents a pure state [3,6].

Although the TDSCF set of equations (20) are classical, the time evolution of the fluctuations $\sigma_{3j} = \langle x_j^2 \rangle - \langle x_j \rangle^2$ and $\sigma_{4j} = \langle p_j^2 \rangle - \langle p_j \rangle^2$ shows that they always satisfy the quantum uncertainty condition. The time evolution of σ_{3j} and σ_{4j} for liquid (V_m = 29.283, T = 89.834 K) and solid (V_m = 28.096, T = 50.275 K) argon using the Lennard-Jones potential are shown in Figs. 2 and 3, respectively.

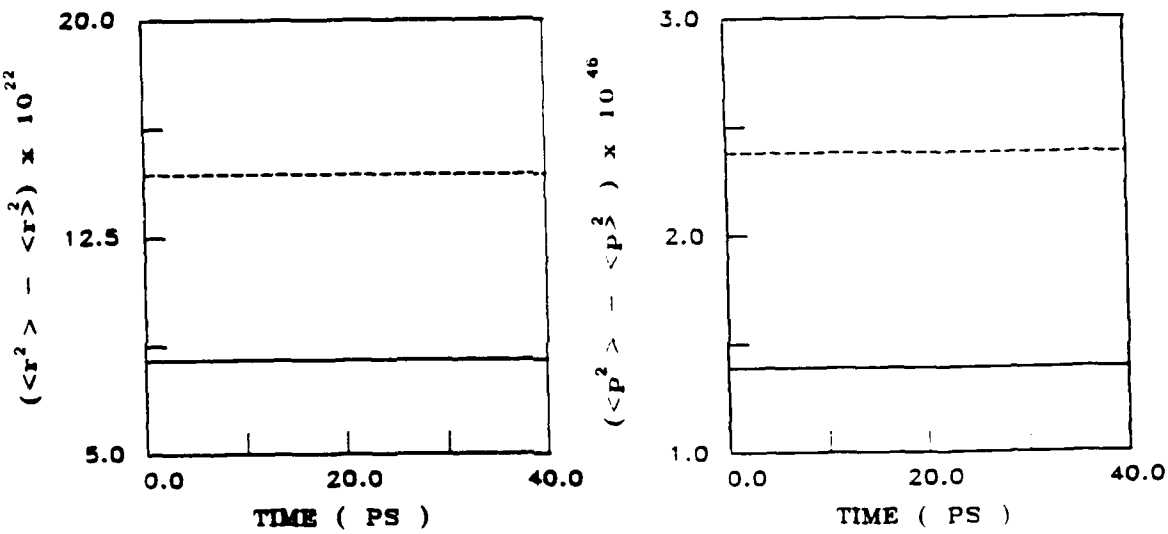

Fig. 2. Time evolution of the dynamical variable $\sigma_3(t) = \sum_{i=1}^{3} \sigma_3^i(t)$ in the units 10^{-22} m^2 obtained by solving Eq. (20) using the predictor algorithm for liquid (---) and solid (–) argon at the temperatures 89.834 K and 50.275 K, respectively, and over a time period of 40 ps. $\sigma_3^i(t)$ represents the position fluctuation along the i-th direction of phase space and averaged over the entire bath.

Fig. 3. The same caption as for Fig. 2, but replacing σ_3 with σ_4 on the vertical axis with the units 10^{-46} $kg^2m^2s^{-2}$.

In general, we observe that the magnitudes of the fluctuations always satisfy

$$\sigma_{3j}\sigma_{4j} - G \geq \frac{\hbar^2}{4} \qquad j = 1, 2, \ldots, 3N \quad , \tag{34}$$

where the magnitude of G is directly proportional to the energy ($\langle E \rangle$) of the system. This in turn suggests that if we have a system such that the fluctuations satisfy condition (34), then its time differentiation yields

$$\dot{\sigma}_{3j}\sigma_{4j} + \dot{\sigma}_{4j}\sigma_{3j} = 0 \qquad j = 1, 2, \ldots, 3N \quad . \tag{35}$$

Since σ_{3j} and σ_{4j} are not zero from the uncertainty condition, one of the possible ways to satisfy (35) would be

$$\dot{\sigma}_{3j} = 0 \qquad j = 1, 2, \ldots, 3N \tag{36a}$$

$$\dot{\sigma}_{4j} = 0 \qquad j = 1, 2, \ldots, 3N \quad . \tag{36b}$$

Combining Eqs. (33) and (36), we obtain a set of equations analogous to (20), except that the choice of the density function is still open in the present case. The density function may be for a single particle or for an N-particle system. Again, the density function may represent a pure state or a mixture. For a Gaussian choice of the density function, our TDSCF set of equations is thus capable of describing the dynamics of all macroscopic and microscopic systems.

DISCUSSION

We have described a method for studying the dynamics of observed reality. The observed system may be classical, classical statistical , quantum, or quantum statistical. The present development is in phase space and thus recovers the trajectory concept even for the microscopic systems. In the present method, the trajectory of a particle is described by a coupled set of equations (12). These equations represent the time evolution of the mean values of position (σ_1) and momentum (σ_2), their fluctuations (diagonal elements of σ_3 and σ_4), their correlations (off-diagonal elements of σ_3, σ_4 and σ_5), and the action terms (diagonal elements of σ_5). The present study has been restricted to isotropic systems, where off-diagonal elements vanish.

The diagonal elements of $\sigma_5(t)$ are identified with action terms since they have units of action and their time evolution is similar to that of the phase terms ($\sigma_5/\hbar$) in the path integral approach. Thus, our present method is reminiscent of Feynman's path integral approach [11], where different values of action correspond to different trajectories. In the path integral method, optimal trajectories are obtained by invoking the classical principle of least action. Inspired by this approach, we have introduced a modified version of the classical principle of least action [Eq. (21)] in the analysis of our results. It is worth noting that, in the present method, the density function contains phase information. In contrast to the path integral approach, the phase vanishes over the minimum action path.

For a Gaussian choice of the density function [Eqs. (17) and (18)], the equations of motion (12) are closed and are completely classical. For an N-particle statistical system, we derived these equations from the quantum Liouville equation using a projection scheme. It was also assumed that the SCF density function approximates the exact density function over all time. This choice of the density function as given in Eq. (3) is similar to the Hartree approximation, where indistinguisability of the particles with respect to their coordinates is ignored.

The concept of indistinguishability in quantum statistics did not originiate from first principles, but rather from the need to explain quantum uncertainty. Indeed, that indistinguishabilty is not inherent in quantum statistics is evident in our model. We characterized each particle with respect to its position and momentum, and their respective fluctuations. The time evolution of the fluctuations allows direct

determination of the quantum uncertainties associated with each particle (Figs. 2 and 3). These fluctuations are constants of motion over the minimum action path ($\delta\sigma_5 = 0$, $\sigma_5 = 0$) and satisfy the quantum uncertainty condition (34). This suggests that indistinguishability is not a must in quantum statistics. Thus, all that is needed to describe an N-particle system is N trajectories with the constraint of minimum action.

It may seem that the validity of this classical description (20) results from the choice of a normalized Gaussian density function [Eqs. (17) and (18)], and therefore the inclusion of higher-order moments would cause a departure from the classical picture. By taking higher-order moments, we introduce fluctuation terms such as $\sigma_i = \langle x_i^3 \rangle - \langle x_i \rangle \langle x_i^2 \rangle - \langle x_i \rangle^3$, which are of third order or greater. Of course, these higher-order terms represent a departure from the Gaussian picture, but, at the same time, go beyond the variances (σ_3, σ_4) defining uncertainty in quantum measurement. Insofar as quantum measurement is random, the choice of a Gaussian density function is appropriate.

Computer simulation shows that the fluctuations in position and momentum of each particle are constants of motion over the minimum action trajectory. Thus, it appears that each particle maintains its distinct trajectory over all time even though the de Broglie wavelengths of individual particles overlap. Insofar as computer simulation suggests that there are N distinct trajectories for an N-particle system, the SCF approximation (3) is vindicated.

The validity of the SCF approximation in turn suggests that an N-particle system is analogous to N interacting wave vectors in a Hilbert space. Measurement on each wavevector then yields the density function ϕ,

$$\phi = \sum_n P_n \, |u_n\rangle \langle u_n| \quad . \tag{37}$$

From the viewpoint of quantum mechanics, the measurement of a dynamical quantity gives various eigenvalues with corresponding eigenvectors $|u_n\rangle$ and probabilities P_n. Measurement, therefore, introduces irreversibility in our microscopic description. Indeed, trajectories obtained from the Schrödinger-Heisenberg picture are indeterministic and consequently time-irreversible. Yet, a phase space (q,p) representation of the density function in Gaussian form (18) recovers the element of time reversibility of measurement (20). Notably, computation of trajectories in our method requires knowledge not only of the position and momentum but also of their fluctuations.

Computed trajectories in the present method are unique since the density function chosen is the one satisfying the maximum entropy principle. This distribution has an important advantage over the canonical distribution ($e^{-\beta H}$) in that the energy constraint condition ($\delta\langle H \rangle = 0$) is eliminated. Our choice of dynamical constraints (15b) in the construction of the density function (15a) makes our theory suitable for nonequilbrium statistical processes. Thus, the present method is far more general than the equilibrium formulations.

In the classical ensemble picture, individual configurations have no significance, whereas in the quantum case it is possible to obtain energy eigenvalues (instead of average energies) for bound state systems, even though the time-energy uncertainty holds. This is because the uncertainty principle imposes restriction only on the product of the uncertainties in

position and momentum (or equivalently energy and time) measurement and not on the individual uncertainties. Relying on this premise and noting that bound states, because of their standing wave nature, have no explicit time dependence, the existence of individual bound energy eigenstates is assumed in the Schrödinger picture. Solution of the corresponding wave equation gives the energy eigenvalues. A striking departure from the classical ensemble picture is thus evident in quantum physics. In the present development the concept of the ensemble picture is retained even in the construction of the density function. Therefore, the concept of eigenstates, which is central to BE and FD statistics, is superfluous in the present method. Further, the symmetry rules of Pauli are implicit in our approach since we do not need explicit knowledge of the probabilities P_n [Eq. (37)]. In order to adapt the present method to Fermions, additional variables are necessary to describe the spin orientation associated with each particle. This extension will be reported in the future.

So far, we have confined applications of the present method to statistical systems only. Nevertheless, it is also suitable for studying atomic and molecular systems. Since for an N-particle system we need a priori knowledge of N rather than N^2 density functions, our approach is particularly attractive for large molecular systems. These applications await future studies. In the present method, the kinetic energy (KE) is evaluated from

$$KE = \sum_{j=1}^{3N} \frac{\langle p_j^2 \rangle}{2m_j} = \sum_{j=1}^{3N} \left(\frac{1}{2m_j} (\sigma_{2j})^2 + [\sigma_4]_{jj} \right) \quad . \tag{38}$$

The temperature for a classical system is related to the kinetic energy by the equipartition theorem,

$$\langle KE \rangle = \frac{1}{N} \sum_{j=1}^{3N} \frac{1}{2m_j} (\sigma_{2j})^2 = \frac{3}{2} kT \quad . \tag{39}$$

Because of the appearance of the momentum fluctuation terms σ_4, the appropriate definition of temperature in our approach is yet to be resolved. Here we should note that temperature in Figs. 2 and 3 incorporates the effect of fluctuation.

In summary, the present dynamical description requires knowledge of position, momentum and their respective fluctuations. This does not allow precise measurement of either position or momentum. As a consequence, the Einstein, Podolsky and Rosen paradox [1,4] does not arise.

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